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Materials characterisation tools towards lead-free piezoceramics

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Electro-mechanical materials directly couple applied mechanical stress and generated electrical charge, or conversely, an applied electric field and a resultant mechanical strain. Airbag triggers, ultrasound emitters and receivers for acoustic imaging, nano-positioning systems, and vibrational energy harvesting devices – these are just a small selection of applications built on the use of electro-mechanical coupling materials such as the piezoceramic PZT ($\text{Pb}(\text{Zr}_{1-x}\text{Ti}_x)\text{O}_3$ – 60wt% lead). Within the EU, the allowed maximum concentration of lead is 0.1 wt% in new electronic equipment as of 2006, though PZT based devices are exempt from this rule until practicable substitutions are available. Hence, major research focus is currently on the development of lead-free alternatives to PZT, but it has proven difficult to achieve comparable properties. A prime reason for the difficulties in replacing PZT is that the electro-mechanical coupling cannot be predicted from material composition and microstructure; the behaviour is complex and multi-length-scale in nature and its exact origins are still a matter of debate.

We have developed 3D grain mapping techniques that enables us to measure changes in microstructure for hundreds of individual grains within the polycrystalline electro-mechanical materials as a function of applied electrical field. The methods are based high energy X-ray diffraction and give access to information on grain positions, sizes, shapes, neighbour relations, phases, crystallographic orientations, strains and volume fractions of the so-called ferroelectric domains. This implies that – for the first time – interactions between neighbouring grains or domains in the polycrystalline electro-mechanical materials can be probed, and the data can be used to directly validate and improve current models describing the electro-mechanical response of ceramic materials. For a more complete picture of the microstructure, X-ray CT can be used to obtain complimentary information on material inhomogeneity and porosity. Examples of using the above 3D characterisation techniques to aid the design and development of new lead-free piezoceramic materials will be presented.

Figure 1 Piezoceramic microstructure: (a) 3D grain map of BaTiO_3 , colours reflect individual grain orientations, and (b) pore structure in $(\text{Ba}_{0.85}\text{Ca}_{0.15})(\text{Zr}_{0.1}\text{Ti}_{0.9})\text{O}_3$ of potential use as bone implant.

